Semiclassical limit for mixed states with singular and rough potentials

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Abstract

We consider the semiclassical limit for the Heisenberg-von Neumann equation with a potential which consists of the sum of a repulsive Coulomb potential, plus a Lipschitz potential whose gradient belongs to BV; this assumption on the potential guarantees the well posedness of the Liouville equation in the space of bounded integrable solutions. We find sufficient conditions on the initial data to ensure that the quantum dynamics converges to the classical one. More precisely, we consider the Husimi functions of the solution of the Heisenberg-von Neumann equation, and under suitable assumptions on the initial data we prove that they converge, as $\varepsilon \to 0$, to the unique bounded solution of the Liouville equation (locally uniformly in time).

1 Introduction

The aim of this paper is to study the semiclassical limit for the Heisenberg-von Neumann (quantum Liouville) equation:

$$\begin{cases} i\varepsilon\partial_t\tilde{\rho}_t^\varepsilon = [H_\varepsilon, \tilde{\rho}_\varepsilon^t], \\ \\ \tilde{\rho}_0^\varepsilon = \tilde{\rho}_{0,\varepsilon}, \end{cases} \tag{1.1}$$

$\{\tilde{\rho}_{0,\varepsilon}\}_{\varepsilon>0}$ being a family of uniformly bounded (with respect to ε), positive, trace class operators, and with $H_\varepsilon = -\frac{\varepsilon^2}{2}\Delta + U$.

When $\tilde{\rho}_{0,\varepsilon}$ is the orthogonal projector onto $\psi_{0,\varepsilon} \in L^2(\mathbb{R}^n)$, (1.2) is equivalent (up to a global phase) to the Schrödinger equation

$$\begin{cases} i\varepsilon\partial_t\psi_t^\varepsilon = -\frac{\varepsilon^2}{2}\Delta\psi_t^\varepsilon + U\psi_t^\varepsilon = H_\varepsilon\psi_t^\varepsilon, \\ \\ \psi_0^\varepsilon = \psi_{0,\varepsilon} \in L^2(\mathbb{R}^n), \end{cases} \tag{1.2}$$

We recall that the Wigner transform $W_\varepsilon\psi$ of a function $\psi \in L^2(\mathbb{R}^n)$ is defined as

$$W_\varepsilon\psi(x,p) := \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \psi(x+\frac{\varepsilon}{2}y)\overline{\psi(x-\frac{\varepsilon}{2}y)}e^{-ipy}dy,$$

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and the one of a density matrix $\tilde{\rho}$ is defined as

$$W_\varepsilon \rho(x,p) := \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \rho(x + \frac{\varepsilon}{2}y, x - \frac{\varepsilon}{2}y) e^{-ipy} dy, \tag{1.3}$$

where $\rho(x,x')$ denotes the integral kernel associated to the operator $\tilde{\rho}$.

The weak limit of the Wigner function of the solution of (1.2) or (1.1) has been studied in many articles (e.g. [15, 13, 14], and more recently in strong topology in [6, 7]). More precisely, it is well-known that the limit dynamics of the Schrödinger equation is related to the Liouville equation

$$\partial_t \mu + p \cdot \nabla_x \mu - \nabla U(x) \cdot \nabla_p \mu = 0, \tag{1.4}$$

and, roughly speaking, the above results state that:
(A) If U is of class C^2 and there exists a sequence $\varepsilon_k \to 0$ such that $W_{\varepsilon_k}\rho_{0,\varepsilon_k}$ converges in the sense of distribution to some (nonnegative) measure μ_0, then $W_{\varepsilon_k}\rho_t^{\varepsilon_k} \to (\Phi_t)_\#\mu_0$ (the convergence is again in the sense of distribution), where Φ_t is the (unique) flow map associated to the Hamiltonian system

$$\begin{cases} \dot{x} = p, \\ \dot{p} = -\nabla U(x) \end{cases} \tag{1.5}$$

so that $\mu_t := (\Phi_t)_\#\mu_0$ is the unique solution to (1.4) (here and in the sequel, $\#$ denotes the push-forward, so that $\mu_t(A) = \mu_0(\Phi_t^{-1}(A))$ for all $A \subset \mathbb{R}^{2n}$ Borel).
(B) If U is of class C^1 and there exists a sequence $\varepsilon_k \to 0$ such that the curve $t \mapsto W_{\varepsilon_k}\rho_t^{\varepsilon_k}$ converges in the sense of distribution to some curve of (nonnegative) measure $t \mapsto \mu_t$, then μ_t solves (1.4).

In the present paper we want to use some recent results proved in [4, 1] to improve the literature in two directions:

(i) By lowering the regularity assumptions of (A) on the potential in order get convergence results for a more general class of potentials, as described below.

(ii) Get rid of the "after an extraction of a subsequence" argument, due to compactness, used in most of the available proofs where one is unable to uniquely identify the limit. More precisely, in (B) above one needs to take a subsequence along which the whole curve $t \mapsto W_{\varepsilon_k}\rho_t^{\varepsilon_k}$ converges for all t in order to obtain a solution to (1.4). Moreover, the limiting solution may depend on the particular subsequence. In our case we will be able to show that, for a class potential much larger than C^2, once one assumes that the Wigner functions at time $t = 0$ have a limit, then the limit at any other time will converge to a "uniquely identified" solution of (1.4).

The price to pay for the lack of regularity of the potential will be to have some size condition on the initial datum which forbids the possibility of considering pure states. Even more, the Wigner function of the initial datum cannot concentrate at a point, a possibility which might actually enter in conflict with the fact that the underlying flow is not uniquely defined everywhere. Let us mention however that, with extra assumptions on the potential (but still allowing the possibility of not having uniqueness of a classical flow), it is possible to consider concentrating initial Wigner functions, giving rise to atomic measures whose evolution follows the "multicharacteristics" of the flow (see [7]).

As described below, we will nevertheless show that, for general bounded and globally Lipschitz potential associated to locally BV vector fields (in addition to some Coulomb part), the Wigner measure of the solution at any time is the push-forward of the initial one by the Ambrosio-DiPerna-Lions flow [9, 2].

Our method will use extensively the Husimi transforms $\psi \mapsto \tilde{W}_\varepsilon \psi$ and $\rho \mapsto \tilde{W}_\varepsilon \rho$, which we recall are defined in terms of convolution of the Wigner transform with the $2n$-dimensional Gaussian kernel with variance $\varepsilon/2$:

$$\tilde{W}_\varepsilon \psi := (W_\varepsilon \psi) * G_\varepsilon^{(2n)}, \quad \tilde{W}_\varepsilon \rho := (W_\varepsilon \rho) * G_\varepsilon^{(2n)}, \quad G_\varepsilon^{(2n)}(x,p) := \frac{e^{-(|x|^2+|p|^2)/\varepsilon}}{(\pi\varepsilon)^n} = G_\varepsilon^{(n)}(x) G_\varepsilon^{(n)}(p). \tag{1.6}$$

Of course, the asymptotic behaviour of the Wigner and Husimi transform is the same in the limit $\varepsilon \to 0$. However, one of the main advantages of the Husimi transform is that it is nonnegative (see Appendix).

Let us observe that, thanks to (A.8), the L^∞-norm of $\tilde{W}_\varepsilon \psi$ can be estimated using the Cauchy-Schwarz inequality:

$$\tilde{W}_\varepsilon \psi(x,p) \leq \frac{1}{\varepsilon^n} \|\psi\|_{L^2}^2 \|\phi_{x,p}^\varepsilon\|_{L^2}^2 = \frac{\|\psi\|_{L^2}^2}{\varepsilon^n}.$$

However, this estimate blows up as $\varepsilon \to 0$. On the other hand we will prove that, by averaging the initial condition with respect to translations, we can get a uniform estimate as $\varepsilon \to 0$ (Section 3.2). This gives us, for instance, an important family of initial data to which our result and the ones in [1] apply (see also the other examples in Section 3).

2 The main results

2.1 Setting

We are concerned with the derivation of classical mechanics from quantum mechanics, corresponding to the study of the asymptotic behaviour of solutions $\tilde{\rho}_t^\varepsilon$ to the Heisenberg-von Neumann equation

$$\begin{cases} i\varepsilon \partial_t \tilde{\rho}_t^\varepsilon = [H_\varepsilon, \tilde{\rho}_t^\varepsilon] \\ \\ \tilde{\rho}_0^\varepsilon = \tilde{\rho}_{0,\varepsilon}, \end{cases} \tag{2.1}$$

as $\varepsilon \to 0$, where $H_\varepsilon = -\frac{\varepsilon^2}{2}\Delta + U$, and $U : \mathbb{R}^n \to \mathbb{R}$ is of the form $U_b + U_s$ on $\mathbb{R}^n$, where U_s is a repulsive Coulomb potential

$$U_s(x) = \sum_{1 \leq i < j \leq M} \frac{Z_i Z_j}{|x_i - x_j|}, \qquad M \leq n/3,\ x = (x_1, \dots x_M, \bar{x}) \in (\mathbb{R}^3)^M \times \mathbb{R}^{n-3M},\ Z_i > 0,$$

U_b is globally bounded, locally Lipschitz, $\nabla U_b \in BV_{\mathrm{loc}}(\mathbb{R}^n;\mathbb{R}^n)$, and

$$\operatorname*{ess\,sup}_{x\in\mathbb{R}^n} \frac{|\nabla U_b(x)|}{1+|x|} < +\infty.$$

The formal solution of (1.2) is $\tilde{\rho}_t^\varepsilon$, where

$$\tilde{\rho}_t^\varepsilon := e^{-itH_\varepsilon/\varepsilon}\tilde{\rho}_{0,\varepsilon}e^{-itH_\varepsilon/\varepsilon}$$

and its kernel is ρ_t^ε. Moreover, as shown for instance in [15], $W_\varepsilon\rho_t^\varepsilon$ solves in the sense of distributions the equation

$$\partial_t W_\varepsilon\rho_t^\varepsilon + p\cdot\nabla_x W_\varepsilon\rho_t^\varepsilon = \mathscr{E}_\varepsilon(U,\rho_t^\varepsilon), \tag{2.2}$$

where $\mathscr{E}_\varepsilon(U,\rho)$ is given by

$$\mathscr{E}_\varepsilon(U,\rho)(x,p) := -\frac{i}{(2\pi)^n}\int_{\mathbb{R}^n}\left[\frac{U(x+\frac{\varepsilon}{2}y)-U(x-\frac{\varepsilon}{2}y)}{\varepsilon}\right]\rho(x+\frac{\varepsilon}{2}y,x-\frac{\varepsilon}{2}y)e^{-ipy}dy. \tag{2.3}$$

Adding and subtracting $\nabla U(x)\cdot y$ in the term in square brackets and using $ye^{-ip\cdot y} = i\nabla_p e^{-ip\cdot y}$, an integration by parts gives $\mathscr{E}_\varepsilon(U,\rho) = \nabla U(x)\cdot\nabla_p W_\varepsilon\rho + \mathscr{E}'_\varepsilon(U,\rho)$, where $\mathscr{E}'_\varepsilon(U,\rho)$ is given by

$$\mathscr{E}'_\varepsilon(U,\rho)(x,p) := -\frac{i}{(2\pi)^n}\int_{\mathbb{R}^n}\left[\frac{U(x+\frac{\varepsilon}{2}y)-U(x-\frac{\varepsilon}{2}y)}{\varepsilon} - \nabla U(x)\cdot y\right]\rho(x+\frac{\varepsilon}{2}y,x-\frac{\varepsilon}{2}y)e^{-ipy}dy. \tag{2.4}$$

Let $\boldsymbol{b}:\mathbb{R}^{2n}\to\mathbb{R}^{2n}$ be the autonomous divergence-free vector field $\boldsymbol{b}(x,p) := \big(p,-\nabla U(x)\big)$. Then, by the discussion above, $W_\varepsilon\rho_t^\varepsilon$ solves the Liouville equation associated to $\boldsymbol{b}$ with an error term:

$$\partial_t W_\varepsilon\rho_t^\varepsilon + \boldsymbol{b}\cdot\nabla W_\varepsilon\rho_t^\varepsilon = \mathscr{E}'_\varepsilon(U,\rho_t^\varepsilon). \tag{2.5}$$

On the other hand, thanks to (2.2), it is not difficult to prove that $\tilde{W}_\varepsilon\rho_t^\varepsilon$ solves in the sense of distributions the equation

$$\partial_t\tilde{W}_\varepsilon\rho_t^\varepsilon + p\cdot\nabla_x\tilde{W}_\varepsilon\rho_t^\varepsilon = \mathscr{E}_\varepsilon(U,\rho_t^\varepsilon)*G_\varepsilon^{(2n)} - \sqrt{\varepsilon}\nabla_x\cdot[W_\varepsilon\rho_t^\varepsilon*\bar{G}_\varepsilon^{(2n)}], \tag{2.6}$$

where

$$\bar{G}_\varepsilon^{(2n)}(y,q) := \frac{q}{\sqrt{\varepsilon}}G_\varepsilon^{(2n)}(y,q). \tag{2.7}$$

Since $W_\varepsilon\rho_t^\varepsilon$ and $\tilde{W}_\varepsilon\rho_t^\varepsilon$ have the same limit points as $\varepsilon\to 0$, the heuristic idea is that in the limit $\varepsilon\to 0$ all error terms should disappear, and we should be left with the Liouville equation (which describes the classical dynamics)

$$\partial_t\omega_t + \boldsymbol{b}\cdot\nabla\omega_t = 0 \qquad \text{on } \mathbb{R}^{2n}.$$

2.2 Preliminary results on the Liouville equations

Under the above assumptions on U one cannot hope for a general uniqueness result in the space of measures for the Liouville equation, as this would be equivalent to uniqueness for the ODE with vector field $\boldsymbol{b}$ (see for instance [3]). On the other hand, as shown in [1, Theorem 6.1], the equation

$$\begin{cases} \partial_t \omega_t + \boldsymbol{b} \cdot \nabla \omega_t = 0 \\ \\ \omega_0 = \bar{\omega} \in L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}) \text{ and nonnegative,} \end{cases} \tag{2.8}$$

has existence and uniqueness in the space $L^\infty_+([0,T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$. This means that there exist a unique $\mathscr{W} : [0,T] \to L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n})$, nonnegative and such that $\operatorname{ess\,sup}_{t\in[0,T]} \|\mathscr{W}_t\|_{L^1(\mathbb{R}^{2n})} + \|\mathscr{W}_t\|_{L^\infty(\mathbb{R}^{2n})} < +\infty$, that solves (2.8) in the sense of distributions on $[0,T] \times \mathbb{R}^{2n}$.

One may wonder whether, in this general setting, solutions to the transport equation can still be described using the theory of characteristics. Even if in this case one cannot solve uniquely the ODE, one can still prove that there exists a unique flow map in the "Ambrosio-DiPerna-Lions sense". Let us recall the definition of *Regular Lagrangian Flow* (in short RLF) in the sense of Ambrosio-DiPerna-Lions:

We say that a (continuous) family of maps $\Phi_t : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$, $t \geq 0$, is a RLF associated to (1.5) if:

- Φ_0 is the identity map.
- For $\mathscr{L}^{2n}$-a.e. (x,p), $t \mapsto \Phi_t(x,p)$ is an absolutely continuous curve solving (1.5).
- For every $T > 0$ there exists a constant C_T such that $(\Phi_t)_\# \mathscr{L}^{2n} \leq C_T \mathscr{L}^{2n}$ for all $t \in [0,T]$,

where $\mathscr{L}^{2n}$ denotes the Lebesgue measure on $\mathbb{R}^{2n}$.
Observe that, since ∇U is not Lipschitz, a priori the ODE (1.5) could have more than one solution for some initial condition. However, the approach via RLFs allows to get rid of this problem by looking at solutions to (1.5) as a whole, and under suitable assumptions on U the RLF associated to (1.5) exists, and it is unique in the following sense: assume that Φ^1 and Φ^2 are two RLFs. Then, for $\mathscr{L}^{2n}$-a.e. (x,p), $\Phi^1_t(x,p) = \Phi^2_t(x,p)$ for all $t \in [0,+\infty)$. In particular, as shown in [1, Section 6], the unique solution to (2.8) is given by

$$\omega_t \mathscr{L}^{2n} = (\Phi_t)_\# \big(\bar{\omega} \mathscr{L}^{2n}\big). \tag{2.9}$$

Hence, the idea is that, if we can ensure that any limit point of the Husimi transforms $\tilde{W}_\varepsilon \rho^\varepsilon_t$ give rives to a curve of measure belonging to $L^\infty_+([0,T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$, by the aforementioned result we would deduce that the limit is unique (once the limit initial datum is fixed), and moreover it is transported by the unique RLF. In order to get such a result we need to make some assumptions on the initial data.

2.3 Assumptions on the initial data and main theorem

Let $\{\tilde{\rho}_{0,\varepsilon}\}_{\varepsilon\in(0,1)}$ be a family of initial data which satisfy

$$\tilde{\rho}_{0,\varepsilon} = \tilde{\rho}^*_{0,\varepsilon}, \quad \tilde{\rho}_{0,\varepsilon} \geq 0 \quad \text{and} \quad \operatorname{tr}(\tilde{\rho}_{0,\varepsilon}) = 1 \qquad \forall \varepsilon \in (0,1).$$

Let

$$\tilde\rho_{0,\varepsilon} = \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_j^{(\varepsilon)}, \cdot\rangle \phi_j^{(\varepsilon)}$$

be the spectral decomposition of $\tilde\rho_{0,\varepsilon}$, and denote by $\rho_{0,\varepsilon}$ its integral kernel.

We assume:

$$\sup_{\varepsilon\in(0,1)} \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \|H_\varepsilon \phi_j^{(\varepsilon)}\|^2 < +\infty, \tag{2.10}$$

$$\frac{1}{\varepsilon^n}\tilde\rho_{0,\varepsilon} \le C\,\mathrm{Id}, \tag{2.11}$$

$$\lim_{R\to+\infty} \sup_{\varepsilon\in(0,1)} \int_{\mathbb{R}\setminus B_R^{(n)}} \rho_{0,\varepsilon}(x,x)\,dx = 0, \tag{2.12}$$

and

$$\lim_{R\to+\infty} \sup_{\varepsilon\in(0,1)} \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}\setminus B_R^{(n)}} \mathcal{F}\rho_{0,\varepsilon}\Big(\frac{p}{\varepsilon},\frac{p}{\varepsilon}\Big)\,dp = 0, \tag{2.13}$$

where $B_R^{(n)}$ is the ball of radius R in $\mathbb{R}^n$ and $\mathcal{F}$ is the Fourier transform on $\mathbb{R}^{2n}$, see (A.5). Conditions (2.12) and (2.13) are equivalent to asking that the family of probability measure $\{\tilde W_\varepsilon\rho_{0,\varepsilon}\}_{\varepsilon\in(0,1)}$ is tight (see Appendix). By Prokhorov's Theorem, this is equivalent to the compactness of $\{\tilde W_\varepsilon\rho_{0,\varepsilon}\}_{\varepsilon\in(0,1)}$ with respect to the weak topology of probability measures (i.e., in the duality with $C_b(\mathbb{R}^{2n})$, the space of bounded continuous functions). Hence, up to extracting a subsequence, assumptions (2.12) together with (2.13) is equivalent to the existence of a probability density $\bar\omega$ such that

$$w-\lim_{\varepsilon\to0} \tilde W_\varepsilon\rho_{0,\varepsilon}\mathscr{L}^{2n} = \bar\omega\mathscr{L}^{2n} \in \mathscr{P}\big(\mathbb{R}^{2n}\big), \tag{2.14}$$

where $\mathscr{P}\big(\mathbb{R}^{2n}\big)$ denotes the space of probability measure on $\mathbb{R}^n$. In order to avoid a tedious notation which would result by working with a subsequence ε_k, we will assume that (2.14) holds along the whole sequence $\varepsilon\to0$, keeping in mind that all the arguments could be repeated with an arbitrary subsequence.

Let us observe that condition (2.10) is slightly weaker than $\sup_{\varepsilon\in(0,1)}\mathrm{tr}(H_\varepsilon^2\tilde\rho_{0,\varepsilon}) < +\infty$, as in order to give a sense to the latter we need the operator $H_\varepsilon^2\tilde\rho_\varepsilon^t$ to make sense (at least on a core). Concerning assumption (2.14), let us observe that the hypothesis $\mathrm{tr}(\tilde\rho_{0,\varepsilon}) = 1$ implies that $\tilde W_\varepsilon\rho_{0,\varepsilon} \in \mathscr{P}\big(\mathbb{R}^{2n}\big)$ (see Appendix).

To express in a better and cleaner way the fact that the convergence is uniform in time, we denote by $d_{\mathscr{P}}$ any bounded distance inducing the weak topology in $\mathscr{P}\big(\mathbb{R}^{2n}\big)$. Recall also that Φ_t denotes the unique RLF associated to $\boldsymbol{b}(x,p) = (p, -\nabla U(x))$, so that $(\Phi_t)_\#\big(\bar\omega\mathscr{L}^{2n}\big)$ is the unique nonnegative solution of (2.8) in $L^\infty_+([0,T]; L^1(\mathbb{R}^{2n})\cap L^\infty(\mathbb{R}^{2n}))$.

Theorem 2.1. *Let U be as in Section 2.1. Under the assumptions (2.10), (2.11) and (2.14)*

$$\lim_{\varepsilon\to0}\sup_{[0,T]} d_{\mathscr{P}}(\tilde W_\varepsilon\rho_t^\varepsilon\mathscr{L}^{2n}, (\Phi_t)_\#\big(\bar\omega\mathscr{L}^{2n}\big)) = 0. \tag{2.15}$$

Moreover, if we define $\mathscr{W}_t\mathscr{L}^{2n} = (\Phi_t)_{\#}(\bar{\omega}\mathscr{L}^{2n})$*, for every smooth function* $\varphi \in C_c^\infty(\mathbb{R}^{2n})$ *the map* $t \mapsto \int_{\mathbb{R}^{2n}} \varphi \mathscr{W}_t\, dx\, dp$ *is continuously differentiable, and*

$$\frac{d}{dt}\int_{\mathbb{R}^{2n}} \varphi \mathscr{W}_t\, dx\, dp = \int_{\mathbb{R}^{2n}} \boldsymbol{b} \cdot \nabla \varphi \mathscr{W}_t\, dx\, dp.$$

The rest of the paper will be concerned with the proof of Theorem 2.1. However, before proceeding with the proof, we first provide some example and sufficient conditions for our result to apply.

3 Examples

We will give three types of examples of density matrices satisfying the assumptions of the preceding section, so that Theorem 2.1 applies.

3.1 Average of an orthonormal basis

For simplicity, we set up our first example in the one-dimensional case. In particular, there is no Coulomb interaction (that is, $U = U_b$), since by assumption Coulomb interactions are three-dimensional. We leave to the interested reader the extension to arbitrary dimension (the only difference in the case $U_s \neq 0$ appears when checking assumption (2.10)).

Let us consider the orthonormal basis of $L^2(\mathbb{R})$ given by the (semiclassical) Hermite functions

$$\psi_j^{(\varepsilon)}(x) = \frac{e^{-x^2/2\varepsilon}}{\sqrt{2^j j!}(\pi\varepsilon)^{1/4}} H_j\left(\frac{x}{\sqrt{\varepsilon}}\right), \qquad j \in \mathbb{N},$$

where H_j's are the Hermite polynomials, i.e.

$$H_j(x) = (-1)^j e^{x^2} \frac{d^j}{dx^j} e^{-x^2}.$$

The following holds:

Proposition 3.1. *Let* $\{\mu_j^{(\varepsilon)}\}_{j\in\mathbb{N}}$ *be a sequence of positive numbers, and define the density matrix* ρ_ε *given by*

$$\rho_\varepsilon = \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \langle \psi_j^{(\varepsilon)}, \cdot \rangle \psi_j^{(\varepsilon)}.$$

Assume that

- $0 \leq \mu_j^{(\varepsilon)} \leq C\varepsilon$, $\sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} = 1$;
- $\varepsilon^2 \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} j^2 \leq C < +\infty$;
- $w - \lim_{\varepsilon\to 0} \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \delta(x^2 + p^2 - j\varepsilon) = \bar{\omega}\mathscr{L}^2 \in \mathscr{P}(\mathbb{R}^2)$.

Then (2.10), (2.11), *and* (2.14) *hold.*

Proof. The first assumption is equivalent to (2.11) and the trace-one condition.

Concerning (2.10), using the well-know fact that

$$\varepsilon \frac{d}{dx}\psi_j^{(\varepsilon)} = \sqrt{\frac{\varepsilon}{2}}\left(\sqrt{j}\psi_{j-1}^{(\varepsilon)} - \sqrt{j+1}\psi_{j+1}^{(\varepsilon)}\right),$$

by a simple calculation it follows that

$$\begin{aligned} H_\varepsilon \psi_j^{(\varepsilon)} &= -\frac{\varepsilon^2}{2}\frac{d^2}{dx^2}\psi_j^{(\varepsilon)} + U_b\psi_j^{(\varepsilon)} \\ &= -\frac{\varepsilon}{4}\left(\sqrt{j(j-1)}\psi_{j-2}^{(\varepsilon)} - (2j+1)\psi_j^{(\varepsilon)} + \sqrt{(j+1)(j+2)}\psi_{j+2}^{(\varepsilon)}\right) + U_b\psi_j^{(\varepsilon)}. \end{aligned}$$

Hence

$$\begin{aligned} \|H_\varepsilon \psi_j^{(\varepsilon)}\|^2 &\leq \left[\frac{\varepsilon}{4}\left(\sqrt{j(j-1)} + (2j+1) + \sqrt{(j+1)(j+2)}\right) + \|U_b\|_\infty\right]^2 \\ &\leq C(1+\varepsilon^2 j^2), \end{aligned}$$

and (2.10) follows from the first two assumptions.

Finally, the third assumption implies (2.14) by noticing that

$$w - \lim_{\varepsilon\to 0, j\to\infty, j\varepsilon\to a} \tilde{W}_\varepsilon \psi_j^{(\varepsilon)} = \delta(x^2+p^2-a) \qquad \forall\, a \geq 0$$

(see, for instance, [15, Exemple III.6]). □

3.2 Töplitz case

Let $\phi \in H^2(\mathbb{R}^n;\mathbb{C})$ with $\int_{\mathbb{R}^n} |\phi(x)|^2\,dx = 1$. Given $\epsilon, \varsigma > 0$, for any $w, q \in \mathbb{R}^n$ let $\psi_{w,q}^\varepsilon$ be defined by

$$\psi_{w,q}^\varepsilon(x) := \frac{1}{\varsigma^{n/2}}\phi\left(\frac{x-q}{\varsigma}\right)e^{i\frac{w\cdot x}{\varepsilon}}.$$

Then, using Plancherel theorem, one can easily check that the identity

$$\frac{1}{\varepsilon^n}\int_{\mathbb{R}^{2n}} |\psi_{w,q}^\varepsilon\rangle\langle\psi_{w,q}^\varepsilon|\,dw\,dq = (2\pi)^n \mathrm{Id} \tag{3.1}$$

holds, where $|\psi\rangle\langle\psi|$ is the Dirac notation for the orthogonal projection onto a normalized vector $\psi \in L^2(\mathbb{R}^n)$. Thanks to (3.1) and the fact that orthogonal projectors are nonnegative operators, we immediately obtain the following important estimate: for every nonnegative bounded function $\chi_\varepsilon : \mathbb{R}^{2n} \to \mathbb{R}$, it holds

$$\frac{1}{\varepsilon^n}\int_{\mathbb{R}^{2n}} \chi_\varepsilon(w,q)|\psi_{w,q}^\varepsilon\rangle\langle\psi_{w,q}^\varepsilon|\,dw\,dq \leq \|\chi_\varepsilon\|_\infty (2\pi)^n \mathrm{Id}. \tag{3.2}$$

Set now

$$\tilde{\rho}_{0,\varepsilon} := \int_{\mathbb{R}^{2n}} \chi_\varepsilon(w,q)|\psi_{w,q}^\varepsilon\rangle\langle\psi_{w,q}^\varepsilon|\,dw\,dq, \qquad \varepsilon \in (0,1),$$

where $\{\chi_\varepsilon\}_{\varepsilon\in(0,1)}$ is a family of nonnegative bounded functions such that $\int_{\mathbb{R}^{2n}} \chi_\varepsilon(w,q)\,dw\,dq = 1$, and let S be the singular set of U_s as defined in (4.27) below.

Proposition 3.2. *Let $\varsigma = \varsigma(\varepsilon) = \varepsilon^\alpha$ with $\alpha \in (0,1)$, and assume that*

- $\sup_{\varepsilon\in(0,1)} \|\chi_\varepsilon\|_\infty < +\infty$.
- $w - \lim_{\varepsilon\to 0} \chi_\varepsilon \mathscr{L}^{2n} = \bar{\omega}\mathscr{L}^{2n} \in \mathscr{P}\big(\mathbb{R}^{2n}\big)$
- $\int_{\mathbb{R}^{2n}} \chi_\varepsilon(w,q) \Big(|w|^4 + \frac{1}{\mathrm{dist}(q,S)^2}\Big)\, dw\, dq \le C < +\infty$.

Then (2.10), (2.11), *and* (2.14) *hold for the family of initial data* $\{\tilde{\rho}_{0,\varepsilon}\}_{\varepsilon\in(0,1)}$.

Proof. (2.11) follows from the first assumption and (3.2).

Since $\varsigma = \varepsilon^\alpha$ with $\alpha \in (0,1)$ we have that for all $(w,q) \in \mathbb{R}^{2n}$

$$w - \lim_{\varepsilon\to 0} \tilde{W}_\varepsilon \psi^\varepsilon_{w,q} \mathscr{L}^{2n} = \delta_{(w,q)},$$

see [15, Exemple III.3], and so (2.14) follows from our second assumption.

To show that the third assumption implies (2.10), we notice that in this case (2.10) can be written as follows

$$\int_{\mathbb{R}^{2n}} \chi_\varepsilon(w,q) \langle H_\varepsilon \psi^\varepsilon_{w,q}, H_\varepsilon \psi^\varepsilon_{w,q}\rangle\, dw\, dq < +\infty. \tag{3.3}$$

Since $\alpha < 1$, and $\phi \in H^2(\mathbb{R}^n;\mathbb{C})$, by a simple computation we get

$$\begin{aligned}
\langle H_\varepsilon \psi^\varepsilon_{w,q}, H_\varepsilon \psi^\varepsilon_{w,q}\rangle &\le \frac{\varepsilon^4}{2}\langle \Delta_x \psi^\varepsilon_{w,q}, \Delta_x \psi^\varepsilon_{w,q}\rangle + 2\langle U\psi^\varepsilon_{w,q}, U\psi^\varepsilon_{w,q}\rangle \\
&\le C\big(1+|w|^4\big) + C\int_{\mathbb{R}^n} U(x)^2 \frac{1}{\varsigma^n}\phi^2\left(\frac{x-q}{\varsigma}\right) dx.
\end{aligned}$$

Since U_b is bounded, $|U_s(q)| \le C/\mathrm{dist}(q,S)$, and $\int_{\mathbb{R}^n} |\phi(x)|^2\, dx = 1$, a simple estimate analogous to the one in Section 4.4 shows that (2.10) holds. We leave the details to the interested reader. $\square$

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3.3 Conditions on the Wigner function

Here we consider a general family of density matrices $\{\tilde{\rho}_{0,\varepsilon}\}_{\varepsilon\in(0,1)}$ which satisfies the tightness conditions (2.12) and (2.13) (so that (2.14) is satisfied up to the extraction of a subsequence). In the next proposition we show some simple sufficient conditions on the Wigner functions $\{W_\varepsilon \rho_{0,\varepsilon}\}_{\varepsilon\in(0,1)}$ in order to ensure the validity of assumptions (2.10) and (2.11).

Proposition 3.3. *Assume that*

- $\max_{|\alpha|,|\beta|\le[\frac{n}{2}]+1} \|\partial_x^\alpha \partial_p^\beta W_\varepsilon \rho_{0,\varepsilon}\|_\infty \le C < +\infty$,
- $\int_{\mathbb{R}^{2n}} \Big(\frac{|p|^4}{4} + U^2(x) + |p|^2 U(x) - \frac{n\varepsilon^2}{2}\Delta U(x)\Big) W_\varepsilon \rho_{0,\varepsilon}(x,p)\, dx\, dp \le C < +\infty$.

Then (2.10) *and* (2.11) *hold.*

Proof. Let us recall first that the Weyl symbol of an operator $\tilde{\rho}$ of integral kernel $\rho(x,y)$ is, by definition, given by

$$\sigma_\varepsilon(\tilde{\rho})(x,p) := \int_{\mathbb{R}^n} \rho(x+\frac{y}{2}, x-\frac{y}{2}) e^{-iy\cdot p/\varepsilon} dy,$$

that is equal to $(2\pi\varepsilon)^n W_\varepsilon \rho$. Moreover, using (A.3) and (A.4), it holds

$$\operatorname{tr}(\tilde{\rho}) = \int_{\mathbb{R}^{2n}} W_\varepsilon \rho(x,p)\, dx\, dp \tag{3.4}$$

Now, we remark that the first assumption gives (2.11) using Calderón-Vaillancourt Theorem [8].

Concerning (2.10), we will prove that

$$\sup_{\varepsilon\in(0,1)} \operatorname{tr}(H_\varepsilon^2 \tilde{\rho}_{0,\varepsilon}) < +\infty$$

(as observed in Section 2.3, this condition is slightly stronger than (2.10)). To this aim, we first note that

$$H_\varepsilon^2 = \frac{\varepsilon^4}{4}\Delta^2 + U^2 - \frac{\varepsilon^2}{2}\Delta U - \frac{\varepsilon^2}{2} U\Delta. \tag{3.5}$$

Moreover, let us observe that if $\tilde{\rho}_1$ and $\tilde{\rho}_2$ have kernels ρ_1 and ρ_2 respectively, then the kernel associated to the operator $\tilde{\rho}_1\tilde{\rho}_2$ is given by $\int \rho_1(\cdot,z)\rho_2(z,\cdot)\, dz$. By this fact and (3.4), a simple computation shows that the identity

$$\operatorname{tr}(A\rho_\varepsilon) = \int_{\mathbb{R}^{2n}} \sigma_\varepsilon(A)(x,p) W_\varepsilon \rho_{0,\varepsilon}(x,p)\, dx\, dp$$

holds for any "suitable" operator A (here $\sigma_\varepsilon(A)$ is the Weyl symbol of A). Hence, in our case,

$$\operatorname{tr}(H_\varepsilon^2 \tilde{\rho}_\varepsilon) = \int_{\mathbb{R}^{2n}} \sigma_\varepsilon(H_\varepsilon^2)(x,p) W_\varepsilon \rho_{0,\varepsilon}(x,p)\, dx\, dp.$$

We claim that the Weyl symbol of H_ε^2 is

$$\sigma_\varepsilon(H_\varepsilon^2)(x,p) = \frac{|p|^4}{4} + U^2(x) + |p|^2 U(x) - \frac{n\varepsilon^2}{2}\Delta U(x).$$

Indeed, let $f(x,p) := |p|^2 = \sigma_\varepsilon(-\varepsilon^2\Delta)(x,p)$ and $g(x,p) := U(x) = \sigma_\varepsilon(U)(x,p)$. Then, using Moyal expansion,

$$\begin{aligned}
\sigma_\varepsilon(H_\varepsilon^2)(x,p) &= \sigma_\varepsilon\left(\frac{\varepsilon^4}{4}\Delta^2 + U^2 - \frac{\varepsilon^2}{2}\Delta U - \frac{\varepsilon^2}{2}U\Delta\right)(x,p) \\
&= \frac{f(x,p)^2}{4} + g(x,p)^2 + \frac{1}{2} f\sharp g(x,p) + \frac{1}{2} g\sharp f(x,p),
\end{aligned}$$

where by definition

$$h_1\sharp h_2(x,p) := e^{i\frac{\varepsilon}{2}(\partial_x\partial_{p'}-\partial_p\partial_{x'})}h_1(x,p)h_2(x',p')\Big|_{x'=x,p'=p}.$$

In our case, in the expansion of the exponential

$$e^{i\frac{\varepsilon}{2}(\partial_x\partial_{p'}-\partial_p\partial_{x'})} = \sum_{j\in\mathbb{N}}\frac{1}{j!}\left(i\frac{\varepsilon}{2}(\partial_x\partial_{p'}-\partial_p\partial_{x'})\right)^j$$

we can stop at the second order term, since $f(x,p)=|p|^2$. Therefore

$$f\sharp g(x,p) = |p|^2U(x) - i\varepsilon p\cdot\nabla U(x) - \frac{n\varepsilon^2}{2}\Delta U(x),$$

and

$$g\sharp f(x,p) = |p|^2U(x) + i\varepsilon p\cdot\nabla U(x) - \frac{n\varepsilon^2}{2}\Delta U(x).$$

This proves the claim and conclude the proof of the proposition.

□

4 Proof of Theorem 2.1

The proof of the theorem is split into several steps: first we show some basic estimates on the solutions, and we prove that the family $\tilde{W}_\varepsilon\rho_t^\varepsilon$ is tight in space and uniformly weakly continuous in time (this is the compactness part). Then we show that $\tilde{W}_\varepsilon\rho_t^\varepsilon$ solves the Liouville equation (away from the singular set of the Coulomb potential) with an error term which converges to zero as $\varepsilon\to 0$. Combining this fact with some uniform decay estimate for $\tilde{W}_\varepsilon\rho_t^\varepsilon$ away from the singularity, we finally prove that any limit point is bounded and solves the Liouville equation. By the uniqueness of solution to the Liouville equation in the function space $L^\infty_+([0,T];L^1(\mathbb{R}^{2n})\cap L^\infty(\mathbb{R}^{2n}))$, we conclude the desired result.

Let us observe that some of our estimates can be found [5] and [1]. However, the setting and the notation there are slightly different, and in some cases one would have to recheck the details of the proofs in [5, 1] to verify that everything works also in our case. Hence, for sake of completeness and in order to make this paper more accessible, we have decided to include all the details.

4.1 Basic estimates

4.1.1 Conserved quantities

The spectral decomposition of $\tilde{\rho}_t^\varepsilon$ is

$$\tilde{\rho}_t^\varepsilon = \sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\langle\phi_{j,t}^{(\varepsilon)},\cdot\rangle\phi_{j,t}^{(\varepsilon)},$$

where $\phi_{j,t}^{(\varepsilon)} = e^{-itH_\varepsilon/\varepsilon}\phi_j^{(\varepsilon)}$ solves (1.2). By standard results on the unitary propagator $e^{-itH_\varepsilon/\varepsilon}$ follows that

$$\sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_{j,t}^{(\varepsilon)}, H_\varepsilon \phi_{j,t}^{(\varepsilon)} \rangle = \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_j^{(\varepsilon)}, H_\varepsilon \phi_j^{(\varepsilon)} \rangle \tag{4.1}$$

and

$$\sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \| H_\varepsilon \phi_{j,t}^{(\varepsilon)} \|^2 = \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \| H_\varepsilon \phi_j^{(\varepsilon)} \|^2 \tag{4.2}$$

for all $t \in \mathbb{R}$ and $\varepsilon \in (0,1)$. Therefore, using (2.10) we have

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in\mathbb{R}} \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_{j,t}^{(\varepsilon)}, H_\varepsilon \phi_{j,t}^{(\varepsilon)} \rangle < +\infty, \tag{4.3}$$

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in\mathbb{R}} \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \| H_\varepsilon \phi_{j,t}^{(\varepsilon)} \|^2 < +\infty. \tag{4.4}$$

4.1.2 A priori estimates

From (4.1), (4.2) and from the fact that $U_s > 0$ and $U_b \in L^\infty(\mathbb{R}^n)$, follows that for all $\varepsilon \in (0,1)$

$$\sup_{t\in\mathbb{R}} \int_{\mathbb{R}^n} U_s^2(x) \rho_t^\varepsilon(x,x)\, dx \le \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \| H_\varepsilon \phi_j^{(\varepsilon)} \|^2 + 2\|U_b\|_\infty \left(\sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_j^{(\varepsilon)}, H_\varepsilon \phi_j^{(\varepsilon)} \rangle + \|U_b\|_\infty \right) \tag{4.5}$$

and

$$\sup_{t\in\mathbb{R}} \frac{1}{2} \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} |\varepsilon \nabla \phi_{j,y}^{(\varepsilon)}(x)|^2\, dx \le \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \langle \phi_j^{(\varepsilon)} H_\varepsilon \phi_j^{(\varepsilon)} \rangle + \|U_b\|_\infty. \tag{4.6}$$

Hence, by (4.3) and (4.4) we obtain

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in\mathbb{R}} \int_{\mathbb{R}^n} U_s^2(x) \rho_t^\varepsilon(x,x)\, dx \le C_1 \tag{4.7}$$

and

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in\mathbb{R}} \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} |\varepsilon \nabla \phi_{j,t}^{(\varepsilon)}(x)|^2\, dx \le C_2. \tag{4.8}$$

4.1.3 Propagation of (2.11) and consequences

Observe that, by unitarity of $e^{itH_\varepsilon/\varepsilon}$, we have, for all $t \in \mathbb{R}$,

$$\frac{1}{\varepsilon^n} \tilde{\rho}_t^\varepsilon \le C\, \mathrm{Id}. \tag{4.9}$$

Hence, since

$$\tilde{W}_\varepsilon \rho_t^\varepsilon(y,p) = \frac{1}{(2\pi)^n} \langle \phi_{y,p}^\varepsilon, \tilde{\rho}_t^\varepsilon \phi_{y,p}^\varepsilon \rangle, \tag{4.10}$$

(see Appendix), using (4.9) we have

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in\mathbb{R}}\|\tilde{W}_\varepsilon\rho_t^\varepsilon\|_\infty \le \frac{C\varepsilon^n}{(2\pi)^n}\|\phi_{y,p}^\varepsilon\|^2 = \frac{C}{(2\pi)^n} \tag{4.11}$$

(because $\|\phi_{y,p}^\varepsilon\| = \varepsilon^{-n/2}$). Now, define for all $x, y \in \mathbb{R}^n$ and $\varepsilon, \lambda > 0$

$$g_{\varepsilon,\lambda,y}(x) = (\sqrt{2}\varepsilon)^{n/2}(\pi\lambda)^{n/4}G^{(n)}_{\lambda\varepsilon^2}(x-y).$$

Observe that

$$\begin{aligned}\frac{1}{\varepsilon^n}\langle g_{\varepsilon,\lambda,y}, \tilde{\rho}_t^\varepsilon g_{\varepsilon,\lambda,y}\rangle &= \frac{1}{\varepsilon^n}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}|\langle g_{\varepsilon,\lambda,y}, \phi_{j,t}^{(\varepsilon))}|^2 \\ &= \frac{1}{\varepsilon^n}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}|(\sqrt{2}\varepsilon)^{n/2}(\pi\lambda)^{n/4}\phi_{j,t}^{(\varepsilon))} * G^{(n)}_{\lambda\varepsilon^2}(y)|^2 \\ &= 2^{n/2}(\pi\lambda)^{n/2}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}|\phi_{j,t}^{(\varepsilon))} * G^{(n)}_{\lambda\varepsilon^2}(y)|^2,\end{aligned}$$

therefore, since $\|g_{\varepsilon,\lambda,y}\| = 1$, by (4.9) we have that

$$2^{n/2}(\pi\lambda)^{n/2}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}|\phi_{j,t}^{(\varepsilon))} * G^{(n)}_{\lambda\varepsilon^2}(y)|^2 \le C. \tag{4.12}$$

So

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\sup_{y\in\mathbb{R}^n}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}|\phi_{j,t}^{(\varepsilon)} * G^{(n)}_{\lambda\varepsilon^2}(y)|^2 \le \frac{C}{\lambda^{n/2}}. \tag{4.13}$$

4.2 Tightness in space

Define $C_R^{(k)} = \{y = (y_1, \dots, y_k) \in \mathbb{R}^k : |y_j| \le R, j = 1, \dots, k\}$. We want to prove that

$$\lim_{R\to+\infty}\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\int_{\mathbb{R}^{2n}\setminus C_R^{(2n)}}\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp = 0. \tag{4.14}$$

Observe that for all $R > 0$

$$\begin{aligned}\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\int_{\mathbb{R}^{2n}\setminus C_R^{(2n)}}\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp \;\le\; &\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\frac{1}{2}\left[\int_{(\mathbb{R}^n\setminus C_R^{(n)})\times\mathbb{R}^n}\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp\right. \\ &\left.+\int_{\mathbb{R}^n\times(\mathbb{R}^n\setminus C_R^{(n)})}\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp\right],\end{aligned}$$

so we can check the tightness property separately for the first and the second marginals of $\tilde{W}_\varepsilon\rho_\varepsilon^t$. From (2.14) follows immediately that the family $\{\tilde{W}_\varepsilon\rho_{\varepsilon,0}\mathscr{L}^{2n}\}_{\varepsilon\in(0,1)}$ is tight (because, by

Prokhorov's Theorem, a family of nonnegative finite measures on $\mathbb{R}^{2n}$ is tight if and only if it is relatively compact in the duality with $C_b(\mathbb{R}^{2n})$). Therefore

$$\lim_{R\to+\infty}\int_{(\mathbb{R}^n\setminus C_R^{(n)})\times\mathbb{R}^n}\tilde{W}_\varepsilon\rho_{\varepsilon,0}(x,p)\,dx\,dp=0. \tag{4.15}$$

Let $\chi\in C(\mathbb{R}^n)$, $0\le\chi\le 1$ such that $\chi(x)=0$ if $|x|<1/2$ and $\chi(x)=1$ if $|x|>1$, and define $\chi_R(x):=\chi(x/R)$. Observe that $\|\nabla\chi_R\|_\infty\le C'/R$ and $\|\Delta\chi_R\|_\infty\le C'/R^2$. We define the following operator:

$$A_R^{(\varepsilon)}\psi(x)=\chi_R*G_\varepsilon^{(n)}(x)\psi(x),\qquad \psi\in L^2(\mathbb{R}^n).$$

Observe that

$$\frac{d}{dt}\mathrm{tr}(A_R^{(\varepsilon)}\tilde{\rho}_\varepsilon^t)=-\frac{i}{\varepsilon}\mathrm{tr}([A_R^{(\varepsilon)},H_\varepsilon]\tilde{\rho}_\varepsilon^t)$$

and that $[A_R^{(\varepsilon)},H_\varepsilon]=\varepsilon^2\big(\Delta(\chi_R*G_\varepsilon^{(n)})/2+\nabla(\chi_R*G_\varepsilon^{(n)})\cdot\nabla\big)$. So, using (4.8),

$$\begin{aligned}\frac{d}{dt}\mathrm{tr}(A_R^{(\varepsilon)}\tilde{\rho}_\varepsilon^t) &= \frac{d}{dt}\int_{\mathbb{R}^{2n}}\chi_R(x)\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp\\ &\le \frac{C'\varepsilon}{R^2}+\frac{C'\sqrt{C_2}}{R}\le\frac{C'}{R^2}+\frac{C'\sqrt{C_2}}{R},\end{aligned}$$

which gives

$$\begin{aligned}\int_{(\mathbb{R}^n\setminus C_{2R}^{(n)})\times\mathbb{R}^n}\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp &\le \int_{\mathbb{R}^{2n}}\chi_R(x)\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp\\ &\le \int_{\mathbb{R}^{2n}}\chi_R(x)\tilde{W}_\varepsilon\rho_{0,\varepsilon}(x,p)\,dx\,dp+\left[\frac{C'}{R^2}+\frac{C'\sqrt{C_2}}{R}\right]T\\ &\le \int_{(\mathbb{R}^n\setminus C_R^{(n)})\times\mathbb{R}^n}\tilde{W}_\varepsilon\rho_{0,\varepsilon}(x,p)\,dx\,dp+\left[\frac{C'}{R^2}+\frac{C'\sqrt{C_2}}{R}\right]T.\end{aligned}$$

Therefore, using (4.15), we get

$$\lim_{R\to+\infty}\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\int_{(\mathbb{R}^n\setminus C_{2R}^{(n)})\times\mathbb{R}^n}\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp=0, \tag{4.16}$$

as desired. For the second marginal we observe first that

$$\int_{\mathbb{R}^{2n}}|p|^2\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp=\int_{\mathbb{R}^{2n}}|p|^2W_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp+\frac{n\varepsilon}{2} \tag{4.17}$$

and

$$\begin{aligned}\int_{\mathbb{R}^{2n}}|p|^2W_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp &= \sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^n}\left|\frac{1}{(2\pi\varepsilon)^{\varepsilon/2}}\hat{\phi}_{j,t}^{(\varepsilon)}\left(\frac{p}{\varepsilon}\right)\right|^2|p|^2\,dp\\ &= \sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^n}|\varepsilon\nabla\phi_{j,t}^{(\varepsilon)}(x)|^2\,dx\end{aligned}$$

therefore, using (4.17) and (4.8), we have that

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\int_{\mathbb{R}^{2n}}|p|^2\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp\le C_2+\frac{n}{2} \tag{4.18}$$

and so

$$0\le\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\int_{\mathbb{R}^n\times(\mathbb{R}^n\setminus C_R^{(n)})}\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp\le\frac{1}{R^2}\Big(C_2+\frac{n}{2}\Big)\to 0\qquad\text{as } R\to+\infty.$$

4.3 Weak Lipschitz continuity in time

Here we prove that for all $\phi\in C_c^\infty(\mathbb{R}^{2n})$ the map

$$t\in\mathbb{R}\mapsto f_{\varepsilon,\phi}(t):=\int_{\mathbb{R}^{2n}}\phi(x,p)\tilde{W}_\varepsilon\rho_t^\varepsilon(x,p)\,dx\,dp$$

is differentiable and

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in\mathbb{R}}\left|\frac{d}{dt}f_{\varepsilon,\phi}(t)\right|\le C_\phi, \tag{4.19}$$

where C_ϕ is a constant depending only on ϕ. First observe that

$$f_{\varepsilon,\phi}(t)=\int_{\mathbb{R}^{2n}}W_\varepsilon\rho_t^\varepsilon(x,p)\phi_\varepsilon(x,p)\,dx\,dp, \tag{4.20}$$

where $\phi_\varepsilon:=\phi*G_\varepsilon^{(2n)}$. Therefore, using (2.2), we have

$$\begin{aligned}\frac{d}{dt}f_{\varepsilon,\phi}(t) &= \int_{\mathbb{R}^{2n}}\mathscr{E}_\varepsilon(U_b,\rho_t^\varepsilon)(x,p)\phi_\varepsilon(x,p)\,dx\,dp\\ &\quad+\int_{\mathbb{R}^{2n}}\mathscr{E}_\varepsilon(U_s,\rho_t^\varepsilon)(x,p)\phi_\varepsilon(x,p)\,dx\,dp\\ &\quad+\int_{\mathbb{R}^{2n}}(p\cdot\nabla_x\phi_\varepsilon(x,p))W_\varepsilon\rho_t^\varepsilon(x,p)\;dx\,dp.\end{aligned} \tag{4.21}$$

For the first term it is easy to check that

$$\left|\int_{\mathbb{R}^{2n}}\mathscr{E}_\varepsilon(U_b,\rho_t^\varepsilon)(x,p)\phi_\varepsilon(x,p)\,dx\,dp\right|\le\frac{\|\nabla U_b\|_\infty}{(2\pi)^n}\int_{\mathbb{R}^n}|y|\sup_{x\in\mathbb{R}^n}|\mathcal{F}_p\phi_\varepsilon|(x,y)\,dy. \tag{4.22}$$

In the case of the Coulomb potential we follow a specific argument borrowed from [5, proof of Theorem 1.1(ii)]), based on the inequality

$$\left|\frac{1}{|z+w/2|}-\frac{1}{|z-w/2|}\right|\le\frac{|w|}{|z+w/2||z-w/2|} \tag{4.23}$$

with $z = (x_i - x_j) \in \mathbb{R}^3$, $w = \varepsilon(y_i - y_j) \in \mathbb{R}^3$. By estimating the difference quotients of U_s as in (4.23), using (4.7) we obtain

$$\begin{aligned} \left| \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_s, \rho_t^\varepsilon)(x,p)\phi_\varepsilon(x,p)\,dx\,dp \right| &\leq C_* \int_{\mathbb{R}^n} |y| \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \phi_\varepsilon(x', y)|\,dy \int_{\mathbb{R}^n} U_s^2(x)\rho_t^\varepsilon(x,x)\,dx \\ &\leq C_* C_1 \int_{\mathbb{R}^n} |y| \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \phi_\varepsilon(x', y)|\,dy, \end{aligned} \tag{4.24}$$

with C_* depending only on the numbers $Z_1, \ldots, Z_M$, and C_1 is the constant defined in (4.7).

For the last term it is easy to see that

$$\left| \int_{\mathbb{R}^{2n}} (p \cdot \nabla_x \phi_\varepsilon(x,p)) W_\varepsilon \rho_t^\varepsilon(x,p)\ dx\,dp \right| \leq \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \tilde{\phi}_\varepsilon|(x', y)\,dy, \tag{4.25}$$

where

$$\tilde{\phi}_\varepsilon(x,p) = p \cdot \nabla_x \phi_\varepsilon(x,p).$$

Therefore we have only to bound

$$\int_{\mathbb{R}^n} |y| \sup_{x \in \mathbb{R}^n} |\mathcal{F}_p \phi_\varepsilon(x,y)|\,dy \quad \text{and} \quad \int_{\mathbb{R}^n} \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \tilde{\phi}_\varepsilon|(x', y)\,dy$$

with a constant depending only on ϕ.

For the first term

$$\begin{aligned} \int_{\mathbb{R}^n} |y| \sup_{x \in \mathbb{R}^n} |\mathcal{F}_p \phi_\varepsilon(x,y)|\,dy &= \int_{\mathbb{R}^n} |y| \sup_{x \in \mathbb{R}^n} \left| \int_{\mathbb{R}^n} G_\varepsilon^{(n)}(x - x') \mathcal{F}_p \phi(x', y)\,dx' \right| |e^{-y^2\varepsilon/4}|\,dy \\ &\leq \int_{\mathbb{R}^n} |y| \sup_{z \in \mathbb{R}^n} |\mathcal{F}_p \phi(z,y)|\ dy \leq C_\phi^{(1)}. \end{aligned}$$

For the second term

$$\int_{\mathbb{R}^n} \sup_{x' \in \mathbb{R}^n} |\mathcal{F}_p \tilde{\phi}_\varepsilon(x', y)|\,dy = \int_{\mathbb{R}^n} \sup_{x \in \mathbb{R}^n} \left| \int_{\mathbb{R}^{3n}} dp\,dx'dp' e^{-ip\cdot y} \phi(x', p') G_\varepsilon^{(n)}(p - p') \left(p \cdot \nabla_x G_\varepsilon^{(n)}(x - x') \right) \right| dy. \tag{4.26}$$

Now observe that

$$\begin{aligned} &\int_{\mathbb{R}^{3n}} dp\,dx'dp' e^{-ip\cdot y} \phi(x', p') G_\varepsilon^{(n)}(p - p') \left(p \cdot \nabla_x G_\varepsilon^{(n)}(x - x') \right) \\ &= \sum_{k=1}^n \int_{\mathbb{R}^{2n}} dx'dp'\ \partial_{x_k} G_\varepsilon^{(n)}(x - x') G_\varepsilon^{(n)}(p') \int_{\mathbb{R}^n} dp\ p_k \phi(x', p - p') e^{-ip\cdot y} \\ &= e^{-\varepsilon y^2/4} \left[\int_{\mathbb{R}^n} dx'\ (\nabla_x \cdot \mathcal{F}_p g(x - x', y)) G_\varepsilon^{(n)}(x') \right. \\ &\quad \left. + \frac{i\varepsilon}{2} \int_{\mathbb{R}^{2n}} dx'\ (y \cdot \nabla_x \mathcal{F}_p \phi(x - x', y)) G_\varepsilon^{(n)}(x') \right], \end{aligned}$$

where $g(x,p) = p\phi(x,p)$. Now, since $\varepsilon \in (0,1)$

$$\begin{aligned}
\int_{\mathbb{R}^n} \sup_{x'\in\mathbb{R}^n} |\mathcal{F}_p \tilde{\phi}_\varepsilon(x',y)|\, dy &\le \int_{\mathbb{R}^n} \sup_{x\in\mathbb{R}^n} \left| \int_{\mathbb{R}^n} dx' \, (\nabla \cdot \mathcal{F}_p g(x-x',y)) G_\varepsilon^{(n)}(x') \right| \\
&\quad + \frac{\varepsilon}{2} \int_{\mathbb{R}^n} \sup_{x\in\mathbb{R}^n} \left| \int_{\mathbb{R}^{2n}} dx' \, (y \cdot \nabla \mathcal{F}_p \phi(x-x',y)) G_\varepsilon^{(n)}(x') \right| \\
&\le \int_{\mathbb{R}^n} dy \, \sup_{z\in\mathbb{R}^n} |\nabla \cdot \mathcal{F}_p g(z,y)| + \frac{\varepsilon}{2} \int_{\mathbb{R}^n} dy \, |y| \sup_{z\in\mathbb{R}^n} |\nabla_z \mathcal{F}_p \phi(z,y)| \\
&\le C_\phi^{(2)}.
\end{aligned}$$

Therefore

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in\mathbb{R}} \left| \frac{d}{dt} f_{\varepsilon,\phi}(t) \right| \le \frac{\|\nabla U_b\|_\infty}{(2\pi)^n} C_\phi^{(1)} + C_* C_1 C_\phi^{(1)} + \frac{C_\phi^{(2)}}{(2\pi)^n}.$$

4.4 Uniform decay away from the singularity

The singular set of U_s is given by

$$S = \bigcup_{1\le i<j\le M} S_{ij}, \quad S_{i,j} = \left\{ x = (x_1,\dots,x_M,\bar{x}) \in (\mathbb{R}^3)^M \times \mathbb{R}^{n-3M} \ : \ x_i = x_j \text{ for some } i \neq j \right\}, \tag{4.27}$$

and we have

$$U_s(x) \ge \frac{c}{\mathrm{dist}(x,S)}, \tag{4.28}$$

where $c > 0$ depending only on $Z_1,\dots,Z_M$. We want to prove that

$$\limsup_{\varepsilon\to 0} \int_{\mathbb{R}^{2n}} \left(|p|^4 + \frac{1}{\mathrm{dist}(x,S)^2} \right) \tilde{W}_\varepsilon \rho_\varepsilon^t(x,p)\, dx\, dp \le C. \tag{4.29}$$

We start with the second term:

$$\begin{aligned}
\int_{\mathbb{R}^{2n}} dx\, dp \frac{1}{\mathrm{dist}(x,S)^2} \tilde{W}_\varepsilon \rho_\varepsilon^t(x,p) &= \int_{B_R^{(n)}\times\mathbb{R}^n} dx\, dx' \frac{\rho_\varepsilon^t(x',x') G_\varepsilon^{(n)}(x-x')}{\mathrm{dist}(x,S)^2} \\
&\le \int_{\mathbb{R}^n} dx' \frac{\rho_\varepsilon^t(x',x')}{\mathrm{dist}(x',S)^2} \\
&\le \frac{1}{c} \int_{\mathbb{R}^n} dx' U_s(x')^2 \rho_\varepsilon^t(x',x') \\
&\le \frac{C_1}{c},
\end{aligned}$$

where c is defined in (4.28), C_1 is defined in (4.7), and we used (4.28).

To prove the second estimate we observe that

$$\int_{\mathbb{R}^{2n}} |p|^4 \tilde{W}_\varepsilon \rho_\varepsilon^t(x,p)\,dx\,dp \le \int_{\mathbb{R}^{2n}} |p|^4 W_\varepsilon \rho_\varepsilon^t(x,p)\,dx\,dp + \frac{n\varepsilon}{2}\int_{\mathbb{R}^{2n}} |p|^2 W_\varepsilon \rho_\varepsilon^t(x,p)\,dx\,dp + \frac{n(n+2)\varepsilon^2}{4}.$$

Thanks to (4.18), it suffices to control the first integral in the right hand side:

$$\begin{aligned}\int_{\mathbb{R}^{2n}} |p|^4 W_\varepsilon \rho_\varepsilon^t(x,p)\,dx\,dp &= \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} \left|\frac{1}{(2\pi\varepsilon)^{\varepsilon/2}} \hat{\phi}_{j,t}^{(\varepsilon)}\left(\frac{p}{\varepsilon}\right)\right|^2 |p|^4\;dp \\ &= \sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} |\varepsilon^2 \Delta \phi_{j,t}^{(\varepsilon)}(x)|^2\;dx \\ &\le 2\sum_{j\in\mathbb{N}} \mu_j^{(\varepsilon)} \int_{\mathbb{R}^n} \left[|H_\varepsilon \phi_{j,t}^{(\varepsilon)}(x)|^2 + U^2(x)|\phi_{j,t}^{(\varepsilon)}(x)|^2\right]\;dx,\end{aligned}$$

and the last term is uniformly bounded thanks to (4.4), (4.7), and the boundedness of U_b.

4.5 Limit continuity equation away from the singularities

We want to prove that

$$\lim_{\varepsilon\to 0} \int_0^T \left[\varphi'(t)\int_{\mathbb{R}^{2n}} \phi(x,p)\tilde{W}_\varepsilon \rho_\varepsilon^t(x,p)\,dx\,dp + \varphi(t)\int_{\mathbb{R}^{2n}} \boldsymbol{b}(x,p)\cdot\nabla\phi(x,p)\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p)\,dx\,dp\right]\;dt = 0 \tag{4.30}$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n}\setminus(S\times\mathbb{R}^n))$ and $\varphi\in C_c^\infty(0,T)$. Hence, recalling (2.6), we have to show that

$$\lim_{\varepsilon\to 0}\sup_{t\in[0,T]} \int_{\mathbb{R}^{2n}} dx\,dp\;\mathscr{E}_\varepsilon(U,\rho_t^\varepsilon) * G_\varepsilon^{(2n)}(x,p)\phi(x,p) + \int_{\mathbb{R}^{2n}} dx\,dp\;\nabla U(x)\cdot\nabla_p\phi(x,p)\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p) = 0, \tag{4.31}$$

and

$$\lim_{\varepsilon\to 0}\int_0^T dt\;\varphi(t)\int_{\mathbb{R}^{2n}} dx\,dp\;\sqrt{\varepsilon}\nabla_x\cdot[W_\varepsilon\rho_t^\varepsilon * \bar{G}_\varepsilon^{(2n)}]\phi(x,p) = 0, \tag{4.32}$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n}\setminus(S\times\mathbb{R}^n))$ and $\varphi\in C_c^\infty(0,T)$.

4.5.1 Verification of (4.31)

We can consider separately the contributions of U_b and U_s. We start with the contribution of U_s. We have to prove that

$$\lim_{\varepsilon\to 0}\sup_{t\in[0,T]} \int_{\mathbb{R}^{2n}} dx\,dp\;\mathscr{E}_\varepsilon(U_s,\rho_t^\varepsilon) * G_\varepsilon^{(2n)}(x,p)\phi(x,p) + \int_{\mathbb{R}^{2n}} dx\,dp\;\nabla U_s(x)\cdot\nabla_p\phi(x,p)\tilde{W}_\varepsilon\rho_\varepsilon^t(x,p) = 0 \tag{4.33}$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n} \setminus (S \times \mathbb{R}^n))$.

We know that

$$\lim_{\varepsilon \to 0} \sup_{t \in [0,T]} \left[\int_{\mathbb{R}^{2n}} \varphi(x,p) W_\varepsilon \rho_\varepsilon^t(x,p)\, dx\, dp - \int_{\mathbb{R}^{2n}} \varphi(x,p) \tilde{W}_\varepsilon \rho_\varepsilon^t(x,p)\, dx\, dp \right] = 0 \tag{4.34}$$

for all $\varphi \in C_c^\infty(\mathbb{R}^{2n})$.

First of all, we see that we can apply (4.34) with $\varphi(x,p) = \nabla U_s(x) \cdot \nabla_p \phi(x,p)$ to replace the integrals

$$\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x,p) \tilde{W}_\varepsilon \psi^\varepsilon \; dx\, dp$$

with

$$\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x,p) W_\varepsilon \psi^\varepsilon \; dx\, dp$$

in the verification of (4.33). Analogously, using (4.7) and (4.24) we see that we can replace

$$\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_s, \rho_\varepsilon^t) * G_\varepsilon^{(2n)}(x,p) \phi(x,p) \; dx\, dp$$

with

$$\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_s, \rho_\varepsilon^t)(x,p) \phi(x,p) \; dx\, dp.$$

Thus, we are led to show the convergence

$$\lim_{\varepsilon \to 0} \sup_{t \in [0,T]} \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_s, \rho_\varepsilon^t) \phi \; dx\, dp + \int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x,p) W_\varepsilon \rho_\varepsilon^t(x,p) \; dx\, dp = 0 \tag{4.35}$$

for all $\phi \in C_c^\infty\big((\mathbb{R}^n \setminus S) \times \mathbb{R}^n\big)$. Since

$$\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_s, \rho_\varepsilon^t) \phi \; dx\, dp = \int_{\mathbb{R}^{2n}} \frac{U_s(x + \frac{\varepsilon}{2} y) - U_s(x - \frac{\varepsilon}{2} y)}{\varepsilon} \rho_\varepsilon^t \left(x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2} \right) \mathcal{F}_p \phi(x,y)\, dx dy$$

we can split the region of integration in two parts, where $\sqrt{\varepsilon}|y| > 1$ and where $\sqrt{\varepsilon}|y| \le 1$. The contribution of the first region can be estimated as in (4.24), with

$$C_* \int_{\{\sqrt{\varepsilon}|y| > 1\}} |y| \sup_{x'} |\mathcal{F}_p \phi(x', y)|\, dy \int_{\mathbb{R}^n} U_s^2(x) \rho_\varepsilon^t(x,x)\, dx,$$

which is infinitesimal, using (4.7) again, as $\varepsilon \to 0$. Since

$$\frac{U_s(x + \frac{\varepsilon}{2} y) - U_s(x - \frac{\varepsilon}{2} y)}{\varepsilon} \to \nabla U_s(x) \cdot y$$

uniformly as $\sqrt{\varepsilon}|y| \le 1$ and x belongs to a compact subset of $\mathbb{R}^n \setminus S$, the contribution of the second part is the same of

$$\int_{\mathbb{R}^{2n}} (\nabla U_s(x) \cdot y) \rho_\varepsilon^t \left(x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2} \right) \mathcal{F}_p \phi(x,y)\, dx dy$$

which coincides with

$$\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x,p) W_\varepsilon \rho_\varepsilon^t(x,p)\ dx\, dp.$$

Now we consider the contribution of U_b. We have to prove that

$$\lim_{\varepsilon\to 0} \sup_{t\in[0,T]} \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b, \rho_\varepsilon^t)(x,p)\phi_\varepsilon(x,p)\ dx\, dp + \int_{\mathbb{R}^{2n}} \nabla U_b(x) \cdot \nabla_p \phi(x,p) \tilde{W}_\varepsilon \rho_t^\varepsilon\ dx\, dp = 0 \quad (4.36)$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n})$, where $\phi_\varepsilon = \phi * G_\varepsilon^{(2n)}$. The proof of (4.36) is divided in two parts: first we prove that

$$\lim_{\varepsilon\to 0} \sup_{t\in[0,T]} \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b, \rho_\varepsilon^t)(x,p)\phi(x,p)\ dx\, dp + \int_{\mathbb{R}^{2n}} \nabla U_b(x) \cdot \nabla_p \phi(x,p) \tilde{W}_\varepsilon \rho_t^\varepsilon\ dx\, dp = 0 \quad (4.37)$$

for all $\phi \in C_c^\infty(\mathbb{R}^{2n})$, and then, using the following estimate

$$\left| \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b, \rho_t^\varepsilon)(x,p)\varphi(x,p)\, dx\, dp \right| \le \frac{\|\nabla U_b\|_\infty}{(2\pi)^n} \int_{\mathbb{R}^n} |y| \sup_{x\in\mathbb{R}^n} |\mathcal{F}_p \varphi|(x,y)\, dy. \quad (4.38)$$

for all $\varphi \in C_c^\infty(\mathbb{R}^{2n})$, we can replace ϕ by ϕ_ε in the first summand of (4.37), obtaining (4.36). The proof of (4.37) is achieved by a density argument. The first remark is that linear combinations of tensor functions $\phi(x,p) = \phi_1(x)\phi_2(p)$, with $\phi_i \in C_c^\infty(\mathbb{R}^n)$, are dense for the norm considered in (4.38). In this way, we are led to prove convergence in the case when $\phi(x,p) = \phi_1(x)\phi_2(p)$. The second remark is that convergence surely holds if U_b is of class C^2 (by the arguments in [15], [5]). Hence, combining the two remarks and using the linearity of the error term with respect to the potential, we can prove convergence by a density argument, by approximating U_b uniformly and in $W^{1,2}$ topology on the support of ϕ_1 by potentials $V_k \in C^2(\mathbb{R}^n)$ with uniformly Lipschitz constants; then, setting $A_k = (U_b - V_k)\phi_1$ and choosing a sequence λ_k in Lemma 4.1 converging slowly to 0 for $k \to +\infty$, in such a way that $\|\nabla A_k\|_2 = o(\lambda_k^{n/4})$ for $k \to +\infty$. In this way we obtain

$$\lim_{k\to\infty} \sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T]} \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b - V_k, \rho_t^\varepsilon)(x,p)\phi_1(x)\phi_2(p)\ dx\, dp = 0.$$

As for the term in (4.36) involving the Husimi transforms, we can use (4.11) to obtain that

$$\begin{aligned} &\limsup_{k\to\infty} \sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T]} \left| \int_{\mathbb{R}^{2n}} \tilde{W}_\varepsilon \rho_t^\varepsilon \nabla(U_b(x) - V_k(x)) \cdot \nabla\phi_2(p)\phi_1(x)\ dx\, dp \right| \\ &\le \frac{C}{(2\pi)^n} \limsup_{k\to\infty} \int_{\mathbb{R}^n} |\phi_1(x)||\nabla U_b(x) - \nabla V_k(x)|\, dx \int_{\mathbb{R}^n} |\nabla\phi_2(p)|\, dp = 0. \end{aligned}$$

So we need only to prove the following lemma:

Lemma 4.1 (A priori estimate). *For all $\lambda > 0$, we have that*

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\left|\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b,\rho_t^\varepsilon)(x,p)\phi_1(x)\phi_2(p)\ dx\,dp\right| \tag{4.39}$$

$$\leq \ \|\phi_1\|_1\|\nabla U_b\|_\infty \sup_{y\in\mathbb{R}^n}|y||\hat{\phi}_2(y)-\hat{\phi}_2 * G_\lambda^{(n)}(y)| + \sqrt{\lambda}\|\nabla A\|_\infty\|\hat{\phi}_2\|_1\int_{\mathbb{R}^n}|u|G_1^{(n)}(u)\,du \tag{4.40}$$

$$+\frac{\sqrt{C}\|\nabla A\|_2}{(2\pi\lambda)^{n/4}}\int_{\mathbb{R}^n}|z||\hat{\phi}_2|(z)\,dz + \|U_b\|_\infty\|\nabla\phi_1\|_\infty\int_{\mathbb{R}^n}|y||\hat{\phi}_2 * G_\lambda^{(n)}|(y)\,dy \tag{4.41}$$

where $A := U_b\phi_1$ and C is the constant in (2.11)*.*

Proof. Set $\hat{\phi}_2 = \mathcal{F}_p\phi_2$. Observe that since (4.38) gives that

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\left|\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b,\rho_t^\varepsilon)\phi_1(x)\phi_2(p)\ dx\,dp - \int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b,\rho_t^\varepsilon)\phi_1(x)\phi_2(p)e^{-|p|^2\lambda}\ dx\,dp\right|$$

$$\leq \ \|\phi_1\|_1\|\nabla U_b\|_\infty \sup_{y\in\mathbb{R}^n}|y||\hat{\phi}_2(y)-\hat{\phi}_2 * G_\lambda^{(n)}(y)|$$

we recognize the first error term in (4.39). So we have only to estimate

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}\left|\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b,\rho_t^\varepsilon)\phi_1(x)\phi_2(p)e^{-|p|^2\lambda}\ dx\,dp\right|. \tag{4.42}$$

Observe that

$$\int_{\mathbb{R}^{2n}} \mathscr{E}_\varepsilon(U_b,\rho_t^\varepsilon)\phi_1(x)\phi_2(p)e^{-|p|^2\lambda}\ dx\,dp = I_{\varepsilon,t} + II_{\varepsilon,t} - III_{\varepsilon,t},$$

where

$$I_{\varepsilon,t} := \int_{\mathbb{R}^{2n}} \frac{A(x+\frac{\varepsilon}{2}y)-A(x-\frac{\varepsilon}{2}y)}{\varepsilon}\hat{\phi}_2 * G_\lambda^{(n)}(y)\rho_t^\varepsilon(x+\frac{\varepsilon}{2}y, x-\frac{\varepsilon}{2}y)\,dxdyd, \tag{4.43}$$

$$II_{\varepsilon,t} := \int_{\mathbb{R}^{2n}} U_b(x+\frac{\varepsilon}{2}y)\frac{\phi_1(x)-\phi_1(x+\frac{\varepsilon}{2}y)}{\varepsilon}\hat{\phi}_2 * G_\lambda^{(n)}(y)\rho_t^\varepsilon(x+\frac{\varepsilon}{2}y, x-\frac{\varepsilon}{2}y)\,dxdy, \tag{4.44}$$

$$III_{\varepsilon,t} := -\int_{\mathbb{R}^{2n}} U_b(x-\frac{\varepsilon}{2}y)\frac{\phi_1(x)-\phi_1(x-\frac{\varepsilon}{2}y)}{\varepsilon}\hat{\phi}_2 * G_\lambda^{(n)}(y)\rho_t^\varepsilon(x+\frac{\varepsilon}{2}y, x-\frac{\varepsilon}{2}y)\,dxdy. \tag{4.45}$$

Observe first that

$$\sup_{\varepsilon\in(0,1)}\sup_{t\in[0,T]}|II_{\varepsilon,t}|+|III_{\varepsilon,t}| \leq \|U_b\|_\infty\|\nabla\phi_1\|_\infty\int_{\mathbb{R}^n}|y||\hat{\phi}_2 * G_\lambda^{(n)}|(y)\,dy.$$

The estimate of $I_{\varepsilon,t}$ is more delicate: we first perform some manipulations of this expression,then we estimate the resulting terms with the help of (4.13).

We expand the convolution product and make the change of variables

$$u = x+\frac{\varepsilon}{2}y \qquad v = x-\frac{\varepsilon}{2}y$$

to get

$$
\begin{aligned}
I_{\varepsilon,t} &= \frac{1}{(\pi\lambda)^{n/2}\varepsilon^n}\int_{\mathbb{R}^{3n}} dudvdz\frac{A(u)-A(v)}{\epsilon}e^{-\frac{|\varepsilon z-(u-v)|^2}{\varepsilon^2\lambda}}\rho_t^\varepsilon(u,v)\hat{\phi}_2(z) \\
&= \frac{1}{\varepsilon}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^{2n}}(A\phi_{j,t}^{(\varepsilon)})*G_{\lambda\varepsilon^2}^{(n)}(v+\varepsilon z)\overline{\phi_{j,t}^{(\varepsilon)}(v)}\hat{\phi}_2(z)\,dvdz \\
&\quad -\frac{1}{\varepsilon}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^{2n}}A(v)(\phi_{j,t}^{(\varepsilon)}*G_{\lambda\varepsilon^2}^{(n)})(v+\varepsilon z)\overline{\phi_{j,t}^{(\varepsilon)}(v)}\hat{\phi}_2(z)\,dvdz \\
&= \frac{1}{\varepsilon}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^{2n}}\Big[(A\phi_{j,t}^{(\varepsilon)})*G_{\lambda\varepsilon^2}^{(n)}(v+\varepsilon z)-A(v+\varepsilon z)(\phi_{j,t}^{(\varepsilon)}*G_{\lambda\varepsilon^2}^{(n)})(v+\varepsilon z)\Big]\overline{\phi_{j,t}^{(\varepsilon)}(v)}\hat{\phi}_2(z)\,dvdz \\
&\quad +\frac{1}{\varepsilon}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^{2n}}[A(v+\varepsilon z)-A(v)]\,(\phi_{j,t}^{(\varepsilon)}*G_{\lambda\varepsilon^2}^{(n)})(v+\varepsilon z)\overline{\phi_{j,t}^{(\varepsilon)}(v)}\hat{\phi}_2(z)\,dvdz. \qquad (4.46)
\end{aligned}
$$

Now let us estimate the first summand in (4.46)

$$
\begin{aligned}
&\left|\frac{1}{\varepsilon}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^{2n}}\Big[(A\phi_{j,t}^{(\varepsilon)})*G_{\lambda\varepsilon^2}^{(n)}(v+\varepsilon z)-A(v+\varepsilon z)(\phi_{j,t}^{(\varepsilon)}*G_{\lambda\varepsilon^2}^{(n)})(v+\varepsilon z)\Big]\overline{\phi_{j,t}^{(\varepsilon)}(v)}\hat{\phi}_2(z)\,dvdz\right| \\
= &\left|\int_{\mathbb{R}^n}dz\,\hat{\phi}_2(z)\int_{\mathbb{R}^{2n}}dudv\,\frac{A(v+\varepsilon z-u)-A(v+\varepsilon z)}{\varepsilon}G_{\lambda\varepsilon^2}^{(n)}(u)\overline{\phi_{j,t}^{(\varepsilon)}(v)}\phi_{j,t}^{(\varepsilon)}(v+\varepsilon z-u)\right| \\
\leq &\ \|\nabla A\|_\infty\int_{\mathbb{R}^n}dz\,|\hat{\phi}_2(z)|\int_{\mathbb{R}^{2n}}dudv\,\frac{|u|}{\varepsilon}G_{\lambda\varepsilon^2}^{(n)}(u)|\overline{\phi_{j,t}^{(\varepsilon)}(v)}||\phi_{j,t}^{(\varepsilon)}(v+\varepsilon z-u)| \\
\leq &\ \sqrt{\lambda}\|\nabla A\|_\infty\|\hat{\phi}_2\|_1\int_{\mathbb{R}^{2n}}|u|G_1^{(n)}(u)\,du.
\end{aligned}
$$

For the second summand in (4.46), using (4.13), we have

$$
\begin{aligned}
&\left|\frac{1}{\varepsilon}\sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^{2n}}[A(v+\varepsilon z)-A(v)]\,(\phi_{j,t}^{(\varepsilon)}*G_{\lambda\varepsilon^2}^{(n)})(v+\varepsilon z)\overline{\phi_{j,t}^{(\varepsilon)}(v)}\hat{\phi}_2(z)\,dvdz\right| \\
\leq &\ \sum_{j\in\mathbb{N}}\mu_j^{(\varepsilon)}\int_{\mathbb{R}^{2n}}\left|\frac{A(v+\varepsilon z)-A(v)}{\varepsilon}\right||(\phi_{j,t}^{(\varepsilon)}*G_{\lambda\varepsilon^2}^{(n)})(v+\varepsilon z)||\overline{\phi_{j,t}^{(\varepsilon)}(v)}||\hat{\phi}_2(z)|\,dvdz \\
\leq &\ \sqrt{\frac{C}{(2\pi\lambda)^{n/2}}}\|\nabla A\|_2\int_{\mathbb{R}^n}|z||\hat{\phi}_2(z)|\,dz.
\end{aligned}
$$

This completes the estimate of the term in (4.43) and the proof. □

4.5.2 Verification of (4.32)

This is easy, taking into account the fact that

$$
\int_{\mathbb{R}^{2n}}W_\varepsilon\rho_\varepsilon^t*\bar{G}_\varepsilon^{(2n)}(x,p)\cdot\nabla_x\phi(x,p)\;dx\,dp=\int_{\mathbb{R}^{2n}}W_\varepsilon\rho_\varepsilon^t\nabla_x\cdot[\phi*\bar{G}_\varepsilon^{(2n)}]\;dx\,dp
$$

are uniformly bounded (recall that $\bar{G}_\varepsilon^{(2n)}$, defined in (2.7), are probability densities).

4.6 Proof of Theorem 2.1

Define $\mathscr{W}^{(\varepsilon)} : [0,T] \to \mathscr{P}\big(\mathbb{R}^{2n}\big)$ as $\mathscr{W}_t^{(\varepsilon)} := \tilde{W}_\varepsilon \rho_\varepsilon^t \mathscr{L}^{2n}$ for all $\varepsilon \in (0,1)$ and $t \in [0,T]$. Using (4.14), (4.19) and Ascoli-Arzelà Theorem, one can prove easily that there exist a subsequence $\big\{\mathscr{W}^{(\varepsilon_k)}\big\}_{k\in\mathbb{N}}$ and $W : [0,T] \to \mathscr{P}\big(\mathbb{R}^{2n}\big)$ such that

$$\lim_{k\to\infty} \sup_{t\in[0,T]} d_{\mathscr{P}}(\mathscr{W}_t^{(\varepsilon_k)}, W_t) = 0. \tag{4.47}$$

We now prove the following assertions:

(i) $W : [0,T] \to \mathscr{P}\big(\mathbb{R}^{2n}\big)$ is weakly continuous and, for all $t \in [0,T]$, $W_t = \tilde{\mathscr{W}}_t \mathscr{L}^{2n}$ for some function $\tilde{\mathscr{W}}_t \in L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n})$. Moreover $\tilde{\mathscr{W}}_t \geq 0$ and $\sup_{t\in[0,T]} \|\tilde{\mathscr{W}}_t\|_{L^1(\mathbb{R}^{2n})} + \|\tilde{\mathscr{W}}_t\|_{L^\infty(\mathbb{R}^{2n})} \leq C$. In particular, $\tilde{\mathscr{W}} \in L^\infty_+([0,T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$.

(ii) $\boldsymbol{b} \in L^1_{\mathrm{loc}}\big((0,T) \times \mathbb{R}^{2n}; dt\, dW_t\big)$, so the continuity equation (2.8) with $\omega_t = \tilde{\mathscr{W}}_t$ makes sense;

(iii) W solves (2.8) in the sense of distributions on $[0,T] \times \mathbb{R}^{2n}$;

(iv) For any $\phi \in C_c^\infty(\mathbb{R}^{2n})$, $t \mapsto \int_{\mathbb{R}^{2n}} \phi\, dW_t$ belongs to $C^1([0,T])$.

Proof of (i): Observe that (4.47) implies that $W : [0,T] \to \mathscr{P}\big(\mathbb{R}^{2n}\big)$ is weakly continuous because it is uniform limit of the weakly continuous maps $\mathscr{W}^{(\varepsilon_k)}$. The second part of the proposition follows immediately from (4.11). Indeed, for all $\phi \in L^1(\mathbb{R}^{2n})$,

$$\sup_{\varepsilon\in(0,1)} \sup_{t\in[0,T]} \int_{\mathbb{R}^{2n}} \phi(x,p) \tilde{W}_\varepsilon \rho_t^\varepsilon(x,p)\; dx\, dp \leq \frac{C}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \phi(x,p)\; dx\, dp \tag{4.48}$$

and so

$$\sup_{t\in[0,T]} \int_{\mathbb{R}^{2n}} \phi(x,p) dW_t(x,p) \leq \frac{C}{(2\pi)^n} \int_{\mathbb{R}^{2n}} \phi(x,p)\; dx\, dp. \tag{4.49}$$

Proof of (ii): The estimate $\boldsymbol{b} \in L^1_{\mathrm{loc}}\big((0,T) \times \mathbb{R}^{2n}; dW_t dt\big)$ follows easily from (4.29) and (4.18).

Proof of (iii): First we prove that $\tilde{\mathscr{W}}$ solves (2.8) in $\mathbb{R}^{2n} \setminus (S \times \mathbb{R}^n)$, where S is the singular set of U_s defined in (4.27). Unfortunately this does not follow immediately by (4.30) because we have no information about the singular set Σ of ∇U_b, so we cannot control the limit $k \to \infty$ of

$$\int_0^T dt\, \varphi(t) \int_{\mathbb{R}^{2n}} dx\, dp\, \nabla U_b(x) \cdot \nabla_p \phi(x,p) \tilde{W}_{\varepsilon_k} \rho_{\varepsilon_k}^t(x,p)$$

in (2.8) with (4.47). But we can proceed by a density argument because, using the regularity conditions (4.48) and (4.49), we can approximate ∇U_b in L^1 on suppϕ by bounded continuous functions.

In order to prove that $\tilde{\mathscr{W}}$ solves (2.8) in $[0,T] \times \mathbb{R}^{2n}$ we use (4.29) to obtain that

$$\sup_{t \in [0,T]} \int_{\mathbb{R}^{2n}} \frac{1}{\mathrm{dist}(x,S)^2} \, dW_t(x,p) \, dt < +\infty. \tag{4.50}$$

Observe that (4.50) implies that $W_t(S \times \mathbb{R}^n) = 0$ for every $t \in (0,T)$. The proof of the global validity of the continuity equation uses the classical argument of removing the singularity by multiplying any test function $\phi \in C_c^\infty(\mathbb{R}^{2n})$ by χ_k, where $\chi_k(x) = \chi(k\mathrm{dist}(x,S))$ and χ is a smooth cut-off function equal to 0 on $[0,1]$ and equal to 1 on $[2,+\infty)$, with $0 \le \chi' \le 2$. If we use $\phi\chi_k$ as a test function, since χ_k depends on x only, we can use the particular structure of $\boldsymbol{b}$, namely $\boldsymbol{b}(x,p) = (p, -\nabla U(x))$, to write the term depending on the derivatives of χ_k as

$$k \int_{\mathbb{R}^{2n}} \phi \chi'(k\mathrm{dist}(x,S)) p \cdot \nabla \mathrm{dist}(x,S) \, dW_t(x,p) dt.$$

If K is the support of ϕ, the integral above can be bounded by

$$2 \sup_K |p\phi| \int_{\{x \in K : k\mathrm{dist}(x,S) \le 2\}} k \, dW_t(x,p) \, dt \le \frac{8 \max_K |p\phi|}{k} \int_K \frac{1}{\mathrm{dist}^2(x,S)} \, dW_t(x,p),$$

and the right hand side is infinitesimal (uniformly in t) as $k \to \infty$.

Proof of (iv): Since the distributional derivative of $t \mapsto \int_{\mathbb{R}^{2n}} \phi W_t \, dx \, dp$ is given by $\int_{\mathbb{R}^{2n}} \boldsymbol{b} \cdot \nabla\phi \, dW_t$, we have to show that the map

$$t \mapsto \int_{\mathbb{R}^{2n}} \boldsymbol{b} \cdot \nabla \phi \, dW_t$$

is continuous. Observing that the map $t \mapsto W_t$ is weakly continuous and $W_t = \tilde{\mathscr{W}}_t \mathscr{L}^{2n}$ with $\tilde{\mathscr{W}} \in L^\infty_+([0,T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$, the only delicate term is

$$\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi(x,p) \, dW_t.$$

Define the nonnegative Hamiltonian function $\mathcal{H} = |p|^2/2 + U + \|U_b\|_\infty$. Taking the limit in (4.29) as $\varepsilon \to 0$ we easily deduce that

$$\sup_{t \in [0,T]} \int_{\mathbb{R}^{2n}} \mathcal{H}^2 \, dW_t \le C \sup_{t \in [0,T]} \int_{\mathbb{R}^{2n}} \Big(1 + |p|^4 + U_s^2(x)\Big) \, dW_t < +\infty.$$

Since the Hamiltonian is preserved by the Liouville dynamics (under our assumptions on the potential, this fact is contained in the proof of [1, Theorem 6.1]), the above bound implies

$$\sup_{t \in [0,T]} \int_{\{\mathcal{H} \ge N\}} \mathcal{H}^2 \, dW_t = \int_{\{\mathcal{H} \ge N\}} \mathcal{H}^2 \, dW_0 \to 0 \qquad \text{as } N \to \infty.$$

As $U_s \le \mathcal{H}$, this implies

$$\sup_{t \in [0,T]} \int_{\{U_s \ge N\}} U_s^2 \, dW_t \le \int_{\{\mathcal{H} \ge N\}} H^2 \, dW_0 \to 0 \qquad \text{as } N \to \infty.$$

Hence, if we define the sets $A_N := \{U_s \le N\}$, the functions

$$t \mapsto f_N(t) := \int_{A_N} \nabla U_s(x) \cdot \nabla_p \phi \, dW_t$$

are continuous and converge uniformly to $\int_{\mathbb{R}^{2n}} \nabla U_s(x) \cdot \nabla_p \phi \, dW_t$ as $N \to \infty$. This proves (iv).

To conclude the proof of the theorem, recalling that $\mathscr{W}$ denote the unique distributional solution of (2.8) in $L^\infty_+([0,T]; L^1(\mathbb{R}^{2n}) \cap L^\infty(\mathbb{R}^{2n}))$ starting from $\bar{\omega}\mathscr{L}^{2n}$ (see [1, Theorem 6.1]), we have proved $\tilde{\mathscr{W}} = \mathscr{W}$, and so

$$\lim_{k\to\infty} \sup_{t\in[0,T]} d_{\mathscr{P}}(\tilde{W}_{\varepsilon_k} \rho^t_{\varepsilon_k} \mathscr{L}^{2n}, \mathscr{W}_t \mathscr{L}^{2n}) = 0. \tag{4.51}$$

Since the limit $\mathscr{W}_t\mathscr{L}^{2n}$ is independent of the chosen subsequence, this implies the convergence of the whole family, namely

$$\lim_{\varepsilon\to 0} \sup_{t\in[0,T]} d_{\mathscr{P}}(\tilde{W}_{\varepsilon} \rho^t_{\varepsilon} \mathscr{L}^{2n}, \mathscr{W}_t \mathscr{L}^{2n}) = 0, \tag{4.52}$$

as desired.

A Notations and some notions about density operators

A density operator on $L^2(\mathbb{R}^n)$ is a positive, self-adjoint, trace-class operator, namely $\tilde{\rho} = \tilde{\rho}^*, \tilde{\rho} \ge 0$ and $\mathrm{tr}(\tilde{\rho}) = 1$, where the trace is defined as follows:

$$\mathrm{tr}(\tilde{\rho}) := \sum_{j\in\mathbb{N}} \langle \varphi_j, \tilde{\rho}\varphi_j \rangle \tag{A.1}$$

with $\{\varphi_j\}_{j\in\mathbb{N}}$ is any orthonormal basis of $L^2(\mathbb{R}^n)$. It can be shown that each density operator $\tilde{\rho}$ is a compact operator, so it can be decomposed as follows

$$\tilde{\rho} = \sum_{j\in\mathbb{N}} \lambda_j \langle \psi_j, \cdot \rangle \psi_j \tag{A.2}$$

where $0 \le \lambda_1 \le \lambda_2 \le \cdots \le 1$, and $\{\psi_j\}_{j\in\mathbb{N}}$ is a orthonormal basis of eigenvectors of $\tilde{\rho}$. Therefore $\tilde{\rho}$ is an integral operator and its kernel is

$$\rho(x,y) = \sum_{j\in\mathbb{N}} \lambda_j \psi_j(x) \overline{\psi_j(y)},$$

so that

$$\tilde{\rho}\psi(x) = \int_{\mathbb{R}^n} \rho(x,y)\psi(y)\, dy.$$

Observe that the trace condition on $\tilde{\rho}$ can be expressed as follows in terms of its kernel

$$\mathrm{tr}(\tilde{\rho}) = \int_{\mathbb{R}^n} \rho(x,x)\, dx = 1. \tag{A.3}$$

The Wigner transform of ρ is defined as

$$W_\varepsilon\rho(x,p) := \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} \rho(x+\frac{\varepsilon}{2}y, x-\frac{\varepsilon}{2}y)e^{-ipy}dy,$$

and the Husimi transform of ρ as

$$\tilde{W}_\varepsilon\rho := W_\varepsilon\rho * G_\varepsilon^{(2n)}, \qquad G_\varepsilon^{(2n)}(x,p) := G_\varepsilon^{(n)}(x)G_\varepsilon^{(n)}(p) = \frac{e^{-\frac{(|x|^2+|p|^2)}{\varepsilon}}}{(\pi\varepsilon)^n}.$$

It is easy to check that the marginals of $W_\varepsilon\rho$ are

$$\int_{\mathbb{R}^n} W_\varepsilon\rho(x,p)\,dp = \rho(x,x) \qquad \text{and} \qquad \int_{\mathbb{R}^n} W_\varepsilon\rho(x,p)\,dx = \frac{1}{(2\pi\varepsilon)^n}\mathcal{F}\left(\frac{p}{\varepsilon},\frac{p}{\varepsilon}\right) \tag{A.4}$$

where

$$\mathcal{F}\rho\,(q,q) = \int_{\mathbb{R}^n} \rho(u,u)e^{-iq\cdot u}\,du. \tag{A.5}$$

Similarly the marginals of $\tilde{W}_\varepsilon\rho$ are

$$\int_{\mathbb{R}^n} \tilde{W}_\varepsilon\rho(x,p)\,dp = \int_{\mathbb{R}^n} \rho(x-x',x-x')G_\varepsilon^{(n)}(x')\,dx' \tag{A.6}$$

and

$$\int_{\mathbb{R}^n} \tilde{W}_\varepsilon\rho(x,p)\,dx = \frac{1}{(2\pi\varepsilon)^n}\int_{\mathbb{R}^n} \mathcal{F}\rho\left(\frac{p-p'}{\varepsilon},\frac{p-p'}{\varepsilon}\right)G_\varepsilon^{(n)}(p')\,dp'. \tag{A.7}$$

Moreover, the Husimi transform is nonnegative: indeed (see for instance [15]),

$$\tilde{W}_\varepsilon\psi(x,p) = \frac{1}{\varepsilon^n}|\langle\psi,\phi_{x,p}^\varepsilon\rangle|^2, \tag{A.8}$$

where $\langle\cdot,\cdot\rangle$ is the scalar product on $L^2(\mathbb{R}^n)$ and

$$\phi_{x,p}^\varepsilon(y) := \frac{1}{(\pi\varepsilon)^{n/4}}e^{-|x-y|^2/(2\varepsilon)}e^{-i(p\cdot y)/\varepsilon} \in L^2(\mathbb{R}^n), \qquad \|\phi_{x,p}^\varepsilon\| = 1.$$

Hence $\tilde{W}_\varepsilon\psi \geq 0$, and using the spectral decomposition (A.2) one obtains the non-negativity of $\tilde{W}_\varepsilon\rho$ for any trace-class operator ρ. Moreover, combining (A.3) and (A.6), it follows that $\tilde{W}_\varepsilon\rho$ is a probability measure.

References

[1] L.Ambrosio, A. Figalli, G. Friesecke, J. Giannoulis, T. Paul : *Semiclassical limit of quantum dynamics with rough potentials and well posedness of transport equations with measure initial data.* arXiv:1006.5388v1, (2010).

[2] L.Ambrosio: *Transport equation and Cauchy problem for BV vector fields.* Invent. Math., **158** (2004), 227–260.

[3] L.Ambrosio: *Transport equation and Cauchy problem for non-smooth vector fields.* Lecture Notes in Mathematics "Calculus of Variations and Non-Linear Partial Differential Equations" (CIME Series, Cetraro, 2005) **1927**, B. Dacorogna, P. Marcellini eds., 2–41, 2008.

[4] L.Ambrosio, A.Figalli: *Almost everywhere well-posedness of continuity equations with measure initial data.* C. R. Math. Acad. Sci. Paris, **348** (2010), no. 5-6, 249–252.

[5] L.Ambrosio, G.Friesecke, J.Giannoulis: *Passage from quantum to classical molecular dynamics in the presence of Coulomb interactions.* Communications in Partial Differential Equations, **35** (2010), 1490-1515.

[6] A.Athanassoulis, T.Paul: *Strong phase-space semiclassical asymptotics.* arXiv:1002.1371v2.

[7] A.Athanassoulis, T.Paul: *Strong and weak semiclassical limits for some rough Hamiltonians* arXiv:1011.1651v2

[8] A.Boulkhemair: *L^2 estimates for Weyl quantization.* J. Funct. Anal., **165** (1999), 173–204.

[9] R.J.DiPerna, P.L.Lions: *Ordinary differential equations, transport theory and Sobolev spaces.* Invent. Math., **98** (1989), 511–547.

[10] Fermanian-Kammerer, P.Gérard: *Mesures semi-classiques et croisement de modes.* Bull. Soc. Math. France, **130** (2002), 123–168.

[11] Fermanian-Kammerer, P.Gérard: *A Landau-Zener formula for non-degenerated involutive codimension 3 crossings.* Ann. Henri Poincaré, **4** (2003), 513–552.

[12] G. Folland: *Harmonic analysis in phase space.* Annals of mathematical studies, **122** (1986), Princeton Univeristy Press.

[13] P.Gérard: *Mesures semi-classiques et ondes de Bloch.* Seminaire sur les Équations aux Dérivées Partielles, 1990-1991. Exp. No. XVI, 19 pp., École Polytechnique, Palaiseau, 1991.

[14] P.Gérard, P.A.Markowich, N.J.Mauser, F.Poupaud: *Homogenization limits and Wigner transforms.* Comm. Pure Appl. Math. **50** (1997), 323–379.

[15] P.L.Lions, T.Paul: *Sur les mesures de Wigner.* Rev. Mat. Iberoamericana, **9** (1993), 553–618.

[16] A.Martinez: *An Introduction to Semiclassical and Microlocal Analysis.* Springer-Verlag, 2002

[17] M.Pulvirenti: *Semiclassical expansion of Wigner functions.* J. Mat. Phys. **47** (2006).

[18] H.Weyl: *The theory of groups and quantum mechanics.* Dover (1931)

[19] E.Wigner: *On the quantum correction for the thermodynamics equilibrium* Phys. Rev **40** (1932) 749-759.

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